



AFRL-AFOSR-VA-TR-2017-0103

Predictive Design of Interfacial Functionality in Polymer Matrix Composites

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**05/24/2017
Final Report**

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REPORT DOCUMENTATION PAGE		Form Approved OMB No. 0704-0188
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1. REPORT DATE (DD-MM-YYYY) 24-05-2017	2. REPORT TYPE Final Performance	3. DATES COVERED (From - To) 01 Nov 2013 to 31 Oct 2016
4. TITLE AND SUBTITLE Predictive Design of Interfacial Functionality in Polymer Matrix Composites		5a. CONTRACT NUMBER 5b. GRANT NUMBER FA9550-14-1-0010
		5c. PROGRAM ELEMENT NUMBER 61102F
6. AUTHOR(S) John Kieffer		5d. PROJECT NUMBER 5e. TASK NUMBER 5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) UNIVERSITY OF MICHIGAN 503 THOMPSON ST ANN ARBOR, MI 48109-1340 US		8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) AF Office of Scientific Research 875 N. Randolph St. Room 3112 Arlington, VA 22203		10. SPONSOR/MONITOR'S ACRONYM(S) AFRL/AFOSR RTA1
		11. SPONSOR/MONITOR'S REPORT NUMBER(S) AFRL-AFOSR-VA-TR-2017-0103
12. DISTRIBUTION/AVAILABILITY STATEMENT A DISTRIBUTION UNLIMITED: PB Public Release		
13. SUPPLEMENTARY NOTES		
14. ABSTRACT <p>With this research we explore interfacial functionality in polymer matrix composites from sensing and monitoring= of mechanical damage to the active control of interfacial phenomena, such as the transport of heat and mass. We use a combined computational and experimental approach. Structures generated using our simulation framework allow us to gain unprecedented insights into anomalous diffusion behavior of water in polyimides and reveal that non-bonding interactions play a more important role in the thermal conductivity of polymers than expected. At 20%-30% of the nominal breakdown voltage we observe small changes in the elastic modulus of PVDF as a result of applying this field, but these changes dissipate with time. Closer inspection of the time dependence of elastic property changes under the influence of external constraints reveal that, as long as the deformation remains within the elastic regime, the elastic modulus gradually returns to the value that corresponds to the unstrained state, presumably as a result of structural reconstitution. Two different relaxation rates govern this process, and they differ by up to two orders of magnitude, depending on the amount of strain applied and the deformation history. The slower processes are only observable in the adiabatic modulus. These results provide insights into the relative magnitudes of entropic and enthalpic changes that occur upon deforming PVDF. We attribute the enthalpic changes predominantly to nonbonding interactions, since in the elastic regime we do not expect covalent bonds to rupture under deformation.</p>		
15. SUBJECT TERMS Interfacial Functionality, Composites, Predictive Design		

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT Unclassified	b. ABSTRACT Unclassified	c. THIS PAGE Unclassified	UU		GORETTA, KENNETH
					19b. TELEPHONE NUMBER (Include area code) 703-696-7349

FINAL REPORT

Project period from 11/01/2015 to 10/31/2016

Project title:

Predictive Design of Interfacial Functionality in Polymer Matrix Composites

AFOSR GRANT NO: FA9550-14-1-0010

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Abstract

With this research we explore interfacial functionality in polymer matrix composites from sensing and monitoring of mechanical damage to the active control of interfacial phenomena, such as the transport of heat and mass. We use a combined computational and experimental approach.

Structures generated using our simulation framework allow us to gain unprecedented insights into anomalous diffusion behavior of water in polyimides and reveal that non-bonding interactions play a more important role in the thermal conductivity of polymers than expected.

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1. Introduction

Interfaces constitute inherent disruptions of the phase character in polymer matrix composites, and due to the thermodynamic mismatch between adjoining components, lead to the formation of extended regions, or interphases, that accommodate the transition between contrasting materials characteristics. Resulting from complex chemical and physical processes during materials fabrication, these interphases often possess less than desirable properties and much effort has been devoted to devising strategies for ameliorating such deterioration. In the proposed research we will make use of interphase formation to supplant this inevitably developing zone with nano-scale and molecular structures that exhibit specific mechanical, thermal, dielectric, and opto-electronic responses, and thereby strategically impart new functionality onto composites.

While the concepts underlying such functionality may be easily derived from known bulk materials properties, realization at the nanoscopic scale afforded by typical interphase domains requires meticulous molecular design and structural manipulation. The ensuing effort may not be easily justified unless sound exploratory evidence exists for its potential success. While in conventional practice the materials design cycle involves the iterative synthesis of materials components in the laboratory, fabrication of a prototype device structure, characterization, property measurements, and the assessment of the device performance. Informed by the measurement findings, the cycle is iterated until either the target outcome is achieved or the concept is abandoned for lack of convergence on this target (Fig. 1). Conversely, the strategic use of simulation to guide experiments allows us to increasing the efficiency of this design cycle (inner loop of Fig. 1). Accordingly, the conception of new interfacial functionality heavily relies on an initial exploration of interface structural responses using simulation tools. This exploratory step is designed to reveal sufficient understanding of the expected behavior before materials are fabricated, thereby deriving a predictive, simulation-based blueprint for molecular architectures with target properties.

2. Objectives

❖ *Establish the integrated computational-experimental framework and research workflow* — that allows us to gain the necessary evidence and procedural insights, based on simulation-based predictive design tools. Molecular simulations will be used to (i) generate realistic models of interfaces and interphase structural design concepts; (ii) determine the functional response of these interphases; (iii) identify the mechanisms underlying their functional response; (iv) predict the achievable response magnitudes of concept interfacial devices for sensing and regulation applications; and (v) experimentally verify the predicted behaviors using proof-of-concept case studies. Accordingly, the project objectives are:

❖ *Gain a better fundamental understanding of interfaces* — in or near their equilibrium constitution, which is essential for the development of optimal structural design criteria. Due to the poor accessibility of interfaces by experimental means, little is known about the molecular definition, defect structures, and local properties at interfaces. Specifically, while the mechanical response of interfacial regions is commonly inferred from their failure behaviors, their elastic properties have so far been elusive due to the difficulties with experimental measurement. Here we employ atomistic simulations and a specialized inelastic light scattering experiment to gain clarity about the pre-failure mechanical response of interfaces and establish the concept of

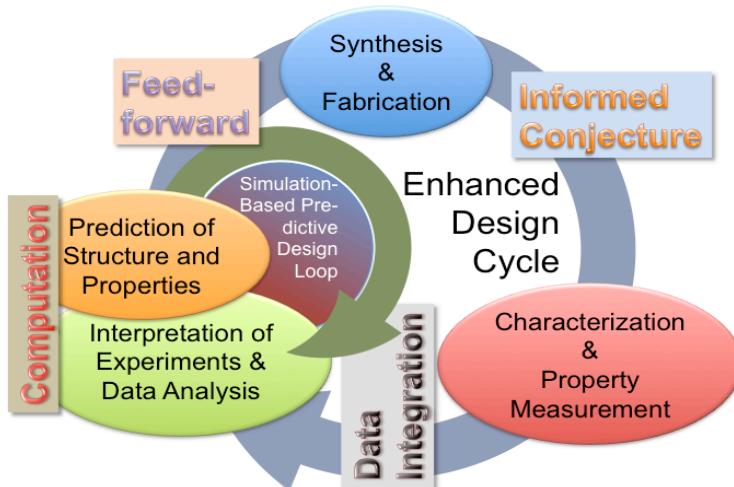


Fig. 1 Schematic of the materials design cycle

interfacial complex elastic moduli. The newly obtained understanding leads to improved composite materials designs, especially with respect to interphase development and properties.

❖ *Devise mechanisms for in-situ monitoring of the structural soundness of interfaces* — in composite materials. Several material properties, e.g., piezoelectricity, thermal and electrical conductivity, refractive indices, and other susceptibilities, are strongly dependent on the structural state of and defect concentrations in the host material. Hence, we are working to create interfacial materials designs capable of sensing impending damage due to fatigue and exposure to deteriorating environmental conditions, (corrosion, radiation, thermal loading, etc.), and of triggering autonomous responses towards damage control and failure prevention.

❖ *Develop useful auxiliary functionality in composites* — such as sensing environmental stimuli, recording application history, energy harvesting, transduction, actuation, and regulation of interfacial properties. For the demonstration of damage sensing interfacial device concepts, the placement of the embedded functional materials component can be targeted at non-load bearing interfaces so as to not interfere with the mechanical integrity of the overall structure. Miniaturized interfacial device layouts allow for space and weight savings. Moreover, new concepts for switching between structural or functional states and thereby controlling thermal, electric, and optical processes at interfaces can be envisioned.

3. Research Approach and Strategy

In this project, computational and experimental research has been undertaken concurrently. On the computational side we have developed algorithms for accelerating polymerization and cross-link reactions in epoxy and polyimide-based materials. These algorithms allow us to generate realistic structural models of polymers near the interfaces with mechanically disparate phases, and to predict the properties and stimuli responses of these interfacial regions in view of discovering and designing new functionalities in composite materials.

We are exploring two mechanisms that would allow us the control thermal transport processes: a change in elastic modulus and a change in adhesive forces. Applying an electric field to an electro-active polymer such as polyvinylidene fluoride (PVDF) induces a strain and the effect of this strain on the polymer structure may result in a change in the elastic modulus. Hence, to rapidly screen the principal materials response underlying thermal transport we measure the elastic properties of PVDF thin films while they are subjected to strong electric fields or other externally applied constraints. Such *in-situ* measurements of the elastic moduli are possible by using the Brillouin light scattering (BLS) technique and by sandwiching the samples between transparent fluoride-doped tin oxide (FTO) glass electrodes to apply the electric fields.

4. Activities during this Project Year

In the previous project year we developed the solution chemistry and the spin coating techniques for the fabrication of PVDF samples in the form of thin films with specific thicknesses, homogeneous quality, and sufficiently large piezoelectric response. We carried out initial measurements of the elastic property changes as a result of an applied field. However, the voltage source we had at our disposal did not provide for the field strengths necessary to observe any effect on the elastic properties of PVDF, and a more powerful high-voltage source was ordered. The new high-voltage source, a Glassman FJ60R2 reversible polarity 60 kV power supply, arrived in fall of 2015 and was integrated into the experimental setup. Now we are able to reach field strengths in excess of the nominal (literature value) breakdown voltage of the material. We repeated the experiments, subjecting samples to higher voltages.

The high-power voltage source setup is designed to allow for concurrent light scattering measurements, which establishes a unique experimental resource. We were able to leverage this new setup with a collaboration in the general context of polymer matrix composite materials, where we studying the alignment of carbon nanotubes (CNT) in epoxy resin *in situ*, by monitoring the orientation-specific CNT Raman bands while an electric field is applied. This work resulted in a publication in 2016.¹

The simulation-based investigation of structure formation in alkane polymers near the interface with a stiff substrate mentioned in previous reports was also published in 2016.²

At moderate field strengths, we started to observe a slight increase in elastic modulus. However, our materials succumbed to dielectric breakdown at much smaller field strengths than those reported in the literature. Again the field strengths we were able to achieve are too small to bring about the elastic modulus changes we are aiming for, but on the other hand, these findings do not disprove the predictions made by our simulations either. The breakdown damage is always very localized, and we conclude that the observed behavior is the result of imperfections in the material. We therefore continue to improve our sample preparation methods so as to achieve more homogeneous and defect free films. In particular we are exploring a new synthesis route that does not require stretching to precipitate the piezoelectric beta-phase.

We also noticed a slight drift in the modulus when subjecting the samples to moderate field strengths for 30 to 40 minutes. This prompted us carry out a detailed investigation of the time dependent behavior of the elastic modulus of PVDF that is subject to mechanical strain, imposed in a way that is easier to control and better defined, i.e., by using a miniature tensile tester that we recently set up on our optical table, so that we are able to measure elastic properties by using conventional stress-strain relationships and BLS simultaneously.

The graduate student, who joined the project in the previous year, Andrew Bielawski, is responsible for the synthesis and fabrication of PVDF films, the sample holder design and implementation, light scattering measurements, as well as data analysis. In the final project year he also embarked on concurrent tensile testing and BLS measurements, for which he joined forces with a new postdoctoral researcher in the group, Dr. Manon Heili, who is working primarily on the AFRL sponsored phase-II SBIR project in collaboration with Advanced Computational Technology (ACT), LLC, of Champaign, IL, and with Elisabeth Woeldgen, an undergraduate student in Aeronautical Engineering at Delft University of Technology in the Netherlands, who spent five weeks during fall of 2015 in our lab as a visiting researcher.

The acquisition and installation of the miniature tensile tester was undertaken to establish a unique experimental resource, independently of any ongoing projects, but it turned out the this AFOSR project was the first to benefit from this new resource. Ms. Woeldgen was brought in to assist with the design calculations associated with the integration of the tensile tester into our optical table layout and beam path, physical construction, and testing of the final configuration.

Finally, another undergraduate student, who has been affiliated with our group for two years, Anthony Fici, has been assisting with chemical synthesis and sample preparation work for this project during the 2015-16 reporting period.

In terms of simulations, Ms. Coyle, continued to investigate the polyimide structure and properties, which primarily serves to establish and refine our predictive simulation framework. However, the choice of system to investigate was made in order to align our efforts with the scope of the collaboration with ACT and AFRL in Dayton, OH. In this project period we focused on the mechanisms of poly-condensation water removal, in particular on analyzing the unique diffusion behavior we observed when the degree of cross-linking reaches significant levels. We also we carried out molecular dynamics studies of thermal transport across simple chain-like polymers, investigating the role of bonding vs. non-bonding interactions.

During 2015-16 PI Kieffer was on sabbatical leave, freed of teaching and service requirements. The majority of time he spent on campus at the University Of Michigan. This allowed him to undertake major improvements with regard to the optical table layout, including the setup of the tensile tester. During this year he was also a visiting professor at the Institut Lumière Matière, Université Claude Bernard Lyon 1, which entailed a one-month long stay in Lyon (June of 2016) to work with the materials physics group on potential collaborations. This group has a large contract with the European Space Agency to work on large telescope optics,

which involves applying hard coatings onto softer substrates, and based on the mutual interests collaborations on interfacial science were initiated.

5. Findings and Outcomes

During this project period we gained new insights into the thermal transport behavior in polymers with various degrees of cross-linking, we observed anomalous diffusion of water in simulation-generated structural models of cross-linked polyimide, and we discovered that in chain-like polymers strained within the elastic regime relaxation of the deformed structure causes its elastic properties to reconstitute, i.e., while the stress-strain relationship would suggest a decrease in elastic modulus upon tensile deformation, the structural relaxation actually results in an increase in the elastic modulus.

❖ Molecular dynamics (MD) simulations allow one to conduct parametric studies, e.g., by continuously varying the strengths of the interactions between molecular constituents, and thereby achieve conditions that are not possible establish in experiments. In this fashion it is also possible to isolate the role of different structural components in defining certain materials properties. In this sense, we investigated the thermal conductivity along the backbone of polymer chains while varying the density, length, and strength of cross-links between the chains. We found that the shorter the cross-links, the stronger the enhancement of thermal conductivity. However, the reason for this behavior is not the increase in mechanical stiffness caused by the cross-links' covalent bonds, but by the increase in non-bonded interactions between chains due to the closer proximity of the polymer backbones achieved by the short ties between them. A manuscript on this aspect is currently under review for publication in the Journal of Physical Chemistry.

❖ We found that water diffusion in polyimide networks is very sensitive to the partial charge attributed to hydrogen and oxygen. An increase in Coulomb interactions tends to slow the diffusion rate. In addition it causes a more pronounced deviation from Brownian motion towards a sub-diffusive behavior, i.e., $\langle r^2 \rangle \propto (2d)\lambda^2\Gamma t^p$ where p is a scaling factor, d is the topological dimension, λ is the average jump distance, and Γ is the effective jump frequency. Sub-diffusive behavior ($0 < p < 1$) is evident from Fig. 2. Anomalous diffusion has been reported experimentally, but no good explanation has been provided thus far in literature for this phenomenon. Generally, one can relate the scaling factor p to the fractal dimension of the diffusion trajectory d_f as $p = 2/d_f$. While super-diffusive behavior ($p > 1$) can be explained as due to a matrix in which migration pathways are spatially restricted, effectively channeling the diffusing species. In the extreme, when $p = 2$ and $d_f = 1$ indicates straight channels. Applying a similar argument to the sub-diffusive behavior would suggest higher dimensional diffusion pathways, i.e., more directions for the molecules to advance into, which effectively slows its progress in any fixed di-

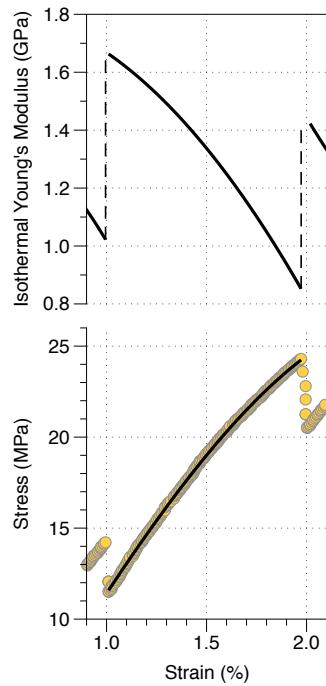


Fig. 3 Stress-strain curve segment for PVDF and isothermal modulus obtained from its derivative.

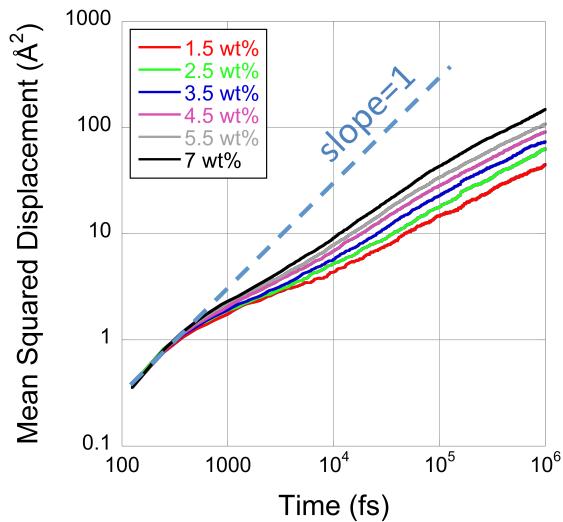


Fig. 2 Mean squared displacements as a function of time on a log-log scale. Deviation from a slope of one indicates anomalous diffusion.

reaction. Of course this approach to interpreting such behaviors is met with difficulty outside to the range $2/3 \leq p \leq 2$, where the trajectory dimensions no longer coincide with conventional concept of space. The polyimide structures we generated provide a unique opportunity to study this phenomenon within a realistic model of an actual materials system.

❖ In our quest to improve the quality of PVDF film, we found that the most consequential factors are the addition of $Mg(NO_3)_2$ hexahydrate to our PVDF/DMF solutions to promote the formation of beta-phase and proper control of the solvent evaporation rate. The latter affects the film quality and beta-phase content. We have discovered a potential source for a new synthesis protocol that results in a large fraction of beta-phase in the as-cast product, i.e., without the need for stretching or poling, developed by a colleague at UM. The protocol will be available to us after the patent disclosure has been filed, but we expect to receive material for testing purposes ahead of time. This development is important in view of fabricating nano-porous PVDF polymer and hybrid materials with large actuation amplitude.

❖ We observe small increases in the elastic modulus of PVDF upon compression effected by moderately high electric field strengths that result in the compression of the films. However, by serendipity we observed what appears to be a creep quality associated with these modulus changes, in that the effect seemed to dissipate with time.

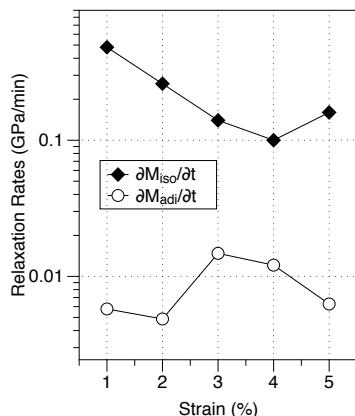


Fig. 2 Relaxation rates of the isothermal and adiabatic longitudinal elastic moduli of PVDF

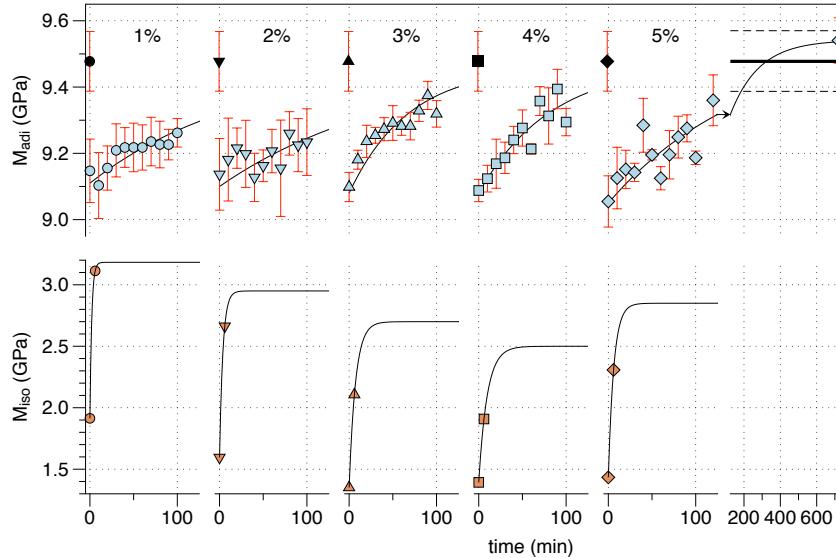


Fig. 4 Timed dependence of the adiabatic (top) and isothermal (bottom) longitudinal elastic moduli of PVDF strained to various degrees (between 1% and 5%) and then held at that strain for two hours. Adiabatic moduli are scaled with respect to the average modulus of all samples before applying the strain (solid black symbols). Data points are fit assuming exponential relaxation with a single rate constant. The last segment shows the relaxation of the modulus for the sample strained to 5% after complete release of this strain.

❖ This observation compelled us to closely examine the time dependence of the changes in the structure and properties of PVDF achieved by external forcing. Because the conditions our PVDF films are subjected to by applying large electric fields are relatively poorly defined, i.e., the field strengths within the material are inhomogeneous, resulting in premature dielectric breakdown, presumably in the vicinity of materials defects, and the strains achieved are small and difficult to quantitatively ascertain, we resorted to use our newly constructed tensile tester sample stage to conduct this study, and imposed strains mechanically.

❖ We strained PVDF to various degrees between 0% and 10%. The latter corresponds to the limit of the range that can safely be considered as elastic. We then held the material at that strain and measured the adiabatic modulus every 10 minutes for about two hours using BLS. The readout from the tensile tester provides the stress-strain relationship, from which we evaluate the isothermal modulus (Fig. 3). As

shown in Fig. 4, the adiabatic modulus is on average about 4.5 times larger than the isothermal modulus. Upon applying the strain, the both moduli drop immediately. However, while held at the imposed strain, the moduli recover, trending towards their values at zero imposed strain, from which we can conclude that the structure of the material reconstitutes while under this constraint. The relaxation rate describing the time dependence of the isothermal modulus is between one and two orders of magnitude faster than that describing the adiabatic modulus (Fig. 5). Note that the isothermal modulus is related to the free energy change of the system due to deformation, while the adiabatic modulus is related to the potential energy change associated with this process. Accordingly, the entropic aspects of the structural deformation recover at least an order of magnitude more rapidly than the enthalpic aspects. A manuscript on this work is currently being prepared.

6. Summary and Outlook

The simulation framework we developed allows us to study the structural developments in polymeric materials, and to gain new insights into interfacial phenomena. These include the pronounced layering and densification in the vicinity of the interphase, the extensive effect of interfacial ordering on elastic properties, and anomalous diffusion behavior in highly cross-linked structures.

At moderate field strengths, approximately 20%-30% of the nominal breakdown voltage, we observe small changes in the elastic modulus of PVDF as a result of applying this field. These changes appear to dissipate with time, although we have not subjected films to strong fields for extended periods of time. Instead, we examined the time dependence of elastic property changes under the influence of external constraints using mechanically induced strains.

The elastic modulus of PVDF decreases upon tensile deformation. As long as the deformation remains within the elastic regime, and while still subject to this strain, the structure of the material reconstitutes, and the elastic modulus gradually returns to the value that corresponds to the unstrained state. (As expected, upon complete strain release, and given enough time, the material reverts to its original state, both in terms of structure and properties.) Two different relaxation rates govern this process, and they differ by up to two orders of magnitude, depending on the amount of strain applied and the deformation history. The slower processes are only observable in the adiabatic modulus. These results provide insights into the relative magnitudes of entropic and enthalpic changes that occur upon deforming PVDF.

We attribute the enthalpic changes predominantly to non-bonding interactions, since in the elastic regime we do not expect covalent bonds to rupture under deformation. This conclusion is consistent with our observations from simulations.

The reconstitution of structure and mechanical properties under strain may limit the effectiveness of changes in elastic moduli as a means to control thermal conduction across boundaries. In the future we will focus our efforts on adhesive forces. Simulations predict that these make a stronger contribution to the effect we seek.

7. Interactions/Transitions:

a. Participation

AFOSR Annual Grantee/Contractor's Meeting on "Low-Density Materials and Microsystems," October 12–14, 2014, Arlington, VA. Oral presentation: "Predictive Design of Interfacial Functionality"

Invited talk at the 2015 Composites at Lake Louise, November 8-12, 2015, Lake Louise, Alberta, Canada, 'Cure kinetics and interfacial phenomena in polymer matrix composites.'

Contributed talk: E. Coyle, K.M. Sebeck, and J. Kieffer, 'Molecular Dynamics Study of Hydration in Amorphous Polyimide,' MRS Fall Meeting, November 19-December 4, 2015, Boston, MA

Contributed talk: A. Bielawski, E. Woeldgen, and J. Kieffer, 'Concurrent Measurement of Adiabatic and Isothermal Elastic Moduli in PVDF under Tensile Strain to Optimize Piezoelectric Response,' MRS Fall Meeting, Nov. 27-Dec. 2, 2016, Boston, MA

Invited talk: A. Bielawski, E. Woeldgen, and J. Kieffer, 'Elastic Deformation and Structural Metrics in Chain-Like Amorphous Polymers,' 2016 Glass & Optical Materials Division Annual Meeting, May 22-26, 2016, Madison, WI.

Contributed talk: V. Rashidi, E. Coyle, J. Kieffer, and K.P. Pipe, 'Engineering thermal conductivity in polymer blends,' APS March Meeting, March 14-18, 2016, Baltimore, MD

Contributed talk: V. Rahsidi, E. Coyle, J. Kieffer, and K.P. Pipe, 'Physical Origins of Thermal Conductivity Enhancements Related to Inter-Chain Bonding in Polymer Blends,' MRS Fall Meeting, Nov. 27-Dec. 2, 2016, Boston, MA

b. Transitions

Continued collaboration with Advanced Computational Technology (ACT), LLC, at Champaign, IL, as a subcontractor on their Phase-II SBIR contract with AFRL in Dayton, OH (Richard Hall, PM). The subject of this SBIR is 'Simulation of Small Scale Damage Evolution During Processing of Polymer Matrix Materials Systems.' Our role is to provide input data to their numerical model based on concurrent Raman and Brillouin light scattering measurements of the mechanical properties of a polyimide during cure.

Initiated a new collaboration on interfacial science with researchers at the Institut Lumière Matière, Université Claude Bernard Lyon 1.

c. Publications and Other Products

- 1 W.A. Chapkin, D.Q. McNerny, M. Aldridge, Y. He, W. Wang, J. Kieffer, and A.I. Taub, 'Real-time assessment of carbon nanotube alignment in a polymer matrix under an applied electric field via polarized Raman spectroscopy,' *Polymer Testing* **56**, 29 (2016).
- 2 C. Sebeck, C. Shao, and J. Kieffer, 'Alkane-Metal Interfacial Structure and Elastic Properties by Molecular Dynamics Simulation,' *ACS Applied Materials and Interfaces* **8**, 16885 (2016).